Self-rotating wave approximation via symmetric ordering of ladder operators

Jonas Larson[1] and Hector Moya-Cessa[2,3]

[1]ICFO-Institute de Cincies Fotoniques, Parc Mediterrani de la Tecnologia, E-08860 Castelldefels (Barcelona)
[2]INAOE, Coordinación de Optica, Apdo. Postal 51 y 216, 72000 Puebla, Pue., México
[3]Universität Ulm, Abteilung für Quantenphysik D-89069 Ulm, Germany

(Dated: February 7, 2008)

We show how some Hamiltonians may be approximated using rotating wave approximation methods. In order to achieve this we use the algebra of boson ladder operators, and transformation formulas between normal and symmetric ordering of the operators. The method presented is studied in two special cases; the Morse and the Mathiue models. The connection with regular perturbation theory is given and the validity of the approximation is discussed.

I. INTRODUCTION

In this contribution we produce approximations for some Hamiltonians such as the ones related with the Morse potential and cosine potential (quantum rotor, or Mathiue differential equation). The approximation is based on the rotating wave approximation (RWA) [1, 2] and symmetric ordering of ladder operators [3]. The RWA is widely used in quantum optical systems and particularly in Jaynes-Cummings types of models [4, 5] and its extensions [6], for example in ion traps [7], cavity quantum electrodynamics [8] and population transfer in atoms and molecules [9]. Also the breakdown of the approximations in similar systems has been considered in several papers [10]. The RWA is usually used for two (or more) interacting subsystems, and in all the above examples, interaction between different subsystems are considered. When passing to the interaction picture with respect to the free Hamiltonian, one remains with a time dependent Hamiltonian that under certain conditions on the frequencies involved may take a simpler form by neglecting terms that oscillate rapidly [2, 4]. A phenomelogical motivation for the approximation is that the neglected terms usually describe non-energy conserving processes, which in the Jaynes-Cummings model discribe simultaneous excitation of the atom/ion and the quantized field. The neglected terms, usually very small within the axperimental parameter regimes, give rise to the Bloch-Siegert shift of the energies [11]. In this paper we show that we can also apply a RWA in a single Hamiltonian systems. Developing the potential in a Taylor series and grouping the quadratic term of the Hamiltonian with the kinetic energy to produce a harmonic oscillator term plus an infinite sum. The frequency of the *artificially produced* harmonic oscillator (HO) is then used as a reference to apply the RWA to the remaining sum. We call this HO a self-HO for the Hamiltonian studied. Using the underlying algebra of the oscillator ladder operators and the RWA, closed forms of the infintie sums are given in two special cases. Only Hamiltonain systems containing bound or quasi bound states may be approximated, and the validity depends on the relative "deepth/width" of the potential; the deeper and narrower potential the better approximation. Thus, it is best suited for low excited bound states, which is verified by numerical simulations. It is also shown that the RWA gives the result of regular first order perturbation theory of the self-HO, which again underlines the validity regimes of the approximation.

We proceed as follows, in the next Section we introduce the self-HO and its Fock states of an arbritary Hamiltonian and derive expressions for the diagonal elements of this Hamiltonian in the Fock basis. This is achieved using the properties of the ladder operators. In sections III and IV, the connection with the RWA is given and two specific models are considered; the Mathieu and Morse equations respectively. The validity of the approximation is investigated in Section V for both studied cases. Secton VI is left for a summery, and in the appendix A is is shown how the methods may be used in a more genaral way for calculating various sums.

II. DIAGONAL MATRIX ELEMENTS IN THE FOCK BASIS OF AN ARBITRARY HAMILTONIAN

Given an arbitrary Hamiltonian we expand the potential term in a Taylor series (in the following we consider for simplicity the case of unit mass and $\hbar = 1$)

$$H = \frac{\hat{p}^2}{2} + V(\hat{x}) = V^{(0)}(0) + V^{(1)}(0)\hat{x} + \frac{\hat{p}^2}{2} + \frac{\omega^2\hat{x}^2}{2} + \sum_{k=3}^{\infty}\frac{V^{(k)}(0)}{k!}\hat{x}^k \tag{1}$$

with $\omega^2 = V^{(2)}(0)$. We let this frequency ω define the ladder operators [12] for the Hamiltonian systems as

$$\hat{a} = \sqrt{\frac{\omega}{2}}\hat{x} + i\frac{\hat{p}}{\sqrt{2\omega}}, \qquad \hat{a}^\dagger = \sqrt{\frac{\omega}{2}}\hat{x} - i\frac{\hat{p}}{\sqrt{2\omega}} \tag{2}$$

The eigenstates of the number operator $N = \hat{a}^\dagger\hat{a}$ is the Fock states, labeled $|N\rangle$. The ladder operators incrase or decrease the quantum number N when acted on a Fock state; $\hat{a}^\dagger|N\rangle = \sqrt{N+1}|N+1\rangle$ and $\hat{a}|N\rangle = \sqrt{N}|n-1\rangle$. Thus, only terms of the infinite sum

$$S = \sum_{k=3}^{\infty} \frac{V^{(k)}(0)}{2^{k/2}k!}\left(\hat{a}^\dagger + \hat{a}\right)^k. \tag{3}$$

of equation (1) that contain an equal number of $\hat{a}^\dagger$:s and $\hat{a}$:s will contribute to the diagonal matrix elements $S_N = \langle N|S|N\rangle$. When considering those elemenst we may therefor neglect all other terms of the sum. We have

$$\left(\hat{a}^\dagger + \hat{a}\right)^k \Rightarrow \begin{cases} \begin{pmatrix} k \\ k/2 \end{pmatrix} : (\hat{a}^\dagger\hat{a})^{k/2} :_W, & k \text{ even} \\ \\ 0 & k \text{ odd} \end{cases} \tag{4}$$

where $: (\hat{a}^\dagger\hat{a})^k :_W$ denotes the Weyl (symmetric) ordering of the operator $\hat{N}^k$. It may be transformed into normal ordering using [13]

$$: (\hat{a}^\dagger\hat{a})^k :_W = \sum_{l=0}^{k} \frac{l!}{2^l}\begin{pmatrix} k \\ l \end{pmatrix}^2 \hat{a}^{\dagger k-l}\hat{a}^{k-l}. \tag{5}$$

Thus, the new sum $\tilde{S}(\hat{x},\hat{p})$, when the "off-diagonal" terms have been neglected (this sum will now depend on the operator $\hat{p}$), may be written as

$$\tilde{S} = \sum_{k=0}^{\infty}\sum_{l=0}^{k} \frac{V^{(2k)}(0)}{2^k(k!)^2}\frac{l!}{2^l}\begin{pmatrix} k \\ l \end{pmatrix}^2 \hat{a}^{\dagger k-l}\hat{a}^{k-l}. \tag{6}$$

The second sum may be taken to infinity (as we may only add zeros)

$$\tilde{S} = \sum_{l=0}^{\infty}\sum_{k=0}^{\infty} \frac{V^{(2k)}(0)}{2^{k+l}(k-l)!^2 l!}\hat{a}^{\dagger k-l}\hat{a}^{k-l}. \tag{7}$$

For $k < l$ the above expression is zero and thus we make the substitution $j = k - l$ and get

$$\tilde{S} = \sum_{l=0}^{\infty} \frac{1}{2^{2l}l!}\sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j(j)!^2}\hat{a}^{\dagger j}\hat{a}^j. \tag{8}$$

By using the identity

$$\hat{a}^{\dagger j}\hat{a}^j = \frac{\hat{N}!}{(\hat{N}-j)!}, \tag{9}$$

the sum is diagonalized in the number basis $\{|N\rangle\}$ and we get the diagonal elements of (1)

$$\langle N|H|N\rangle = \omega(N+\frac{1}{2}) + \sum_{l=0}^{\infty} \frac{1}{2^{2l}l!}\sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j(j)!^2}\frac{N!}{(N-j)!}, \tag{10}$$

where we have used that $\langle N|\hat{p}^2/2|N\rangle = \langle N|\omega^2\hat{x}^2/2|N\rangle = \frac{\omega}{2}(N+\frac{1}{2})$. Note that the Fock basis used to calculate the diagonal elements of the Hamiltonian are obtained from the quadratic term of the Hamiltonian and we call them $|N\rangle$ instead of the usual notation $|n\rangle$. In the following sections we apply the above to some specific examples.

III. COSINE POTENTIAL

Using the fact that we can obtain closed forms for the diagonal elements of some of the potentials studied in Section II, and noting that the RWA is used to keep constant terms (terms that do not rotate), in this Section we show that

for some Hamiltonians we can produce approximations under certain circumstances, namely, when some parameters allow us to perform the RWA.

One very important equation for scientists is the Mathieu equation [14, 15, 16] which is identical to the Schrödinger equation with a sin or cosin potential, also known as the quantum rotor. Durning the last decade it has gained a new shove of attention due to the growing field of cold atoms in optical lattices [17]. Approximate results of the eigenfunctions and eigenvalues of the Mathieu equation have been studied earlier [18, 19, 20]. Known approximation methods from physics, such as the WKB and the Raman-Nath have been applied to the Mathieu equation [19]. Given the Hamiltonian (reminding that we set $\hbar = 1$ and $m = 1$)

$$H = \frac{\hat{p}^2}{2} - g_0^2 \cos q\hat{x} \tag{11}$$

we can expand the cosine as (we neglect the constat term as it only displaces the energies)

$$H = \frac{\hat{p}^2}{2} + \frac{g_0^2 q^2}{2}\hat{x}^2 - g_0^2 \sum_{k=2}^{\infty} \frac{(q\hat{x})^{2k}}{(2k)!}(-1)^k. \tag{12}$$

With the above definition of the creation and annihilation operators (2), we get

$$\hat{a} = \sqrt{\frac{g_0 q}{2}}\hat{x} + i\frac{\hat{p}}{\sqrt{2g_0 q}}, \qquad \hat{a}^\dagger = \sqrt{\frac{g_0 q}{2}}\hat{x} - i\frac{\hat{p}}{\sqrt{2g_0 q}}, \tag{13}$$

and rewrite the Hamiltonian as

$$H = g_0 q(\hat{a}^\dagger\hat{a} + \frac{1}{2}) - g_0^2 \sum_{k=2}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(\hat{a}^\dagger + \hat{a})^{2k}}{(2k)!}(-1)^k \tag{14}$$

In the case $g_0 \gg \frac{q}{4}$ we can do RWA, and thus go to a rotating frame with respect to the free Hamiltonian, $U(t) = \exp\left(-ig_0 q\hat{a}^\dagger\hat{a}t\right)$. Using the relations

$$U^\dagger(t)\hat{a}U(t) = \hat{a}\mathrm{e}^{ig_0qt}, \qquad U^\dagger(t)\hat{a}^\dagger U(t) = \hat{a}^\dagger\mathrm{e}^{-ig_0qt}, \tag{15}$$

and by only keeping non-rotating tyerms in the Hamiltonian we find

$$H = g_0 q\left(\hat{N} + \frac{1}{2}\right) - g_0^2 \sum_{k=2} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k!)^2} : (\hat{a}^\dagger\hat{a})^k :_W \tag{16}$$

We now proced as in section II. Inserting (5) into (16) we have $H = g_0 q\left(\hat{N} - 1/2\right) - g_0^2 S$ with

$$S \equiv \sum_{k=2}^{\infty}\sum_{l=0}^{k} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k!)^2}\frac{l!}{2^l}\begin{pmatrix} k \\ m \end{pmatrix}^2 \hat{a}^{\dagger k-l}\hat{a}^{k-l} \tag{17}$$

Rearranging terms and like in equation (7) we can sum l to infinity to get

$$S = \sum_{l=0}^{\infty}\frac{1}{2^l l!}\sum_{k=2}^{\infty}\left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2}\hat{a}^{\dagger k-l}\hat{a}^{k-l}. \tag{18}$$

By expressing

$$\begin{aligned}\sum_{k=0}^{\infty}\left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2}\hat{a}^{\dagger k-l}\hat{a}^{k-l} &= \sum_{k=2}^{\infty}\left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2}\hat{a}^{\dagger k-l}\hat{a}^{k-l} \\ &+ 1 - \left(\frac{q}{2g_0}\right)\frac{1}{(1-l)!^2}\hat{a}^{\dagger 1-l}\hat{a}^{1-l},\end{aligned} \tag{19}$$

we can write $S = S_1 + S_2$ with

$$S_1 = \sum_{l=0}^{\infty}\frac{1}{2^l l!}\sum_{k=0}^{\infty}\left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2}\hat{a}^{\dagger k-m}\hat{a}^{k-l} \tag{20}$$

and

$$S_2 = \left(\frac{q}{2g_0}\right)(\hat{a}^\dagger\hat{a} + \frac{1}{2}) - 1. \tag{21}$$

Note that, like previous in section II, the second sum in equation (20) may be started at $k = l$, i.e.

$$\begin{aligned} S_1 &= \sum_{l=0}^{\infty} \frac{1}{2^l l!} \sum_{k=l}^{\infty} \left(\frac{q}{2g_0}\right)^k \frac{(-1)^k}{(k-l)!^2} \hat{a}^{\dagger k-l}\hat{a}^{k-l} \\ &= \sum_{l=0}^{\infty} \frac{(-1)^l}{2^l l!} \left(\frac{q}{2g_0}\right)^l \sum_{n=0}^{\infty} \left(\frac{q}{2g_0}\right)^n \frac{(-1)^n}{n!^2} \hat{a}^{\dagger n}\hat{a}^n. \end{aligned} \tag{22}$$

or

$$S_1 = e^{-\frac{\beta}{4g_0}} : J_0\left(\frac{q}{2g_0}\hat{a}^\dagger\hat{a}\right) : \tag{23}$$

or using that $\hat{a}^{\dagger j}\hat{a}^j = \frac{\hat{N}!}{(\hat{N}-j)!}$

$$S_1 = e^{-\frac{q}{4g_0}} L_{\hat{N}}\left(\frac{q}{2g_0}\right) \tag{24}$$

The result obtained here agree with previous results were approximations to the Mathieu equation are obtained [18]. The result also gives an interesting relation between zeroth Bessel function and Laguerre polynomials.

Combining the results we find the diagonalized RWA Hamiltonian

$$H = \frac{g_0 q}{2}\left(\hat{N} + \frac{1}{2}\right) - g_0^2 \mathrm{e}^{-\frac{q}{4g_0}} L_{\hat{N}}\left(\frac{q}{2g_0}\right). \tag{25}$$

If we develop the Laguerre polynomials in powers of q/g_0, which should be valid within the regimes of the RWA, and remain to second order we obtain

$$H \approx g_0 q(\hat{N} + \frac{1}{2}) - \frac{q^2}{16}(\hat{N}^2 + \hat{N} + \frac{1}{2}) - g_0^2. \tag{26}$$

It should also be pointed out that the method also works for superimposed cosine potentials; $\sum_k g_k^2 \cos(q_k x)$. This has interesting applications in for example solid state physics [21] and cold atoms in optical superlattices [22].

We conclude this section by making an analogy betwen the RWA and first order perturbation theory. Given the Hamiltonian

$$H = g_0 q\left(\hat{N} + \frac{1}{2}\right) \tag{27}$$

with eigenstates $|N\rangle$, we perturb it with

$$V = -g_0^2\cos(qx) - \frac{g_0^2 q^2}{2}x^2. \tag{28}$$

The first order corerection to the energy [23] becomes

$$\delta E = \langle\Psi_n|V|\Psi_n\rangle = -g_0^2 \mathrm{e}^{-\frac{q}{4g_0}} L_n\left(\frac{q}{2g_0}\right) - \frac{g_0 q}{2}\left(n + \frac{1}{2}\right), \tag{29}$$

which regains exactly the same result as the one obtained from the RWA method. This relation between first order perturbation theory and the RWA method is easily shown, using Eq. (A4), to be valid in any general case.

IV. MORSE POTENTIAL

Now let us look at the Morse potential [24, 25], from which we get the Hamiltonian

$$H = \frac{\hat{p}^2}{2} + \lambda^2(1 - \exp[-\alpha(\hat{x} - b)])^2 \tag{30}$$

This kind of Hamiltonian is commonly used to describe properties of diatomic molecules and other situation with anharmonicity [26]. The Morse Hamiltonian has turned out to have interesting properties in connection with the WKB approximation [27, 28] (the WKB quantization gives the exact spectrum), and with supersymetric quantum mechanics [29].

One can transform the Hamiltonian by means of the displacement operator $e^{ib\hat{p}}$ so that $H_T = e^{ib\hat{p}} H e^{-ib\hat{p}} = \frac{\hat{p}^2}{2} + \lambda^2(1 - \exp[-\alpha\hat{x}])^2$. The transformed Hamiltonian is then written in the approximate form (we neglect odd powers because of RWA, i.e. we are in the regime $\lambda \gg \alpha$)

$$H = \sqrt{2}\lambda\alpha(\hat{N} + 1/2) + \lambda^2(S_1 + S_2) \tag{31}$$

with

$$S_1 = \sum_{k=2} \frac{(2\alpha\hat{x})^{2k}}{(2k)!}, \qquad S_2 = -2\sum_{k=2} \frac{(\alpha\hat{x})^{2k}}{(2k)!} \tag{32}$$

Following the procedure of the former section we may write

$$S_1 = e^{\frac{\alpha}{\sqrt{2}\lambda}} L_{\hat{N}}(-\frac{\sqrt{2}\alpha}{\lambda}) - \frac{\sqrt{2}\alpha}{\lambda}(\hat{N} + 1/2) - 1 \tag{33}$$

and

$$S_2 = -2\left(e^{\frac{\alpha}{4\sqrt{2}\lambda}} L_{\hat{N}}(-\frac{\alpha}{2\sqrt{2}\lambda}) - \frac{\alpha}{2\sqrt{2}\lambda}(\hat{N} + 1/2) - 1\right) \tag{34}$$

giving the RWA Hamiltonian

$$H = \frac{\sqrt{2}\lambda\alpha}{2}\left(\hat{N} + \frac{1}{2}\right) + \lambda^2 \mathrm{e}^{\frac{\alpha}{\sqrt{2}\lambda}} L_{\hat{N}}\left(-\frac{\sqrt{2}\alpha}{\lambda}\right) - 2\lambda^2 \mathrm{e}^{\frac{\alpha}{4\sqrt{2}\lambda}} L_{\hat{N}}\left(-\frac{\alpha}{2\sqrt{2}\lambda}\right) + \lambda^2. \tag{35}$$

Using the fact that $\lambda \gg \alpha$ in the RWA validity regime, we expand the Hamiltonian to second order in α/λ

$$H \approx \frac{3}{4}\sqrt{2}\lambda\alpha\left(\hat{N} + \frac{1}{2}\right) + \frac{7\alpha^2}{16}\left(\hat{N}^2 + \hat{N} + \frac{1}{2}\right). \tag{36}$$

Note that if we write the (transformed) Morse Hamiltonian as

$$H = \sqrt{2}\lambda\alpha(\hat{N} + 1/2) + \lambda^2(1 - \exp[-\frac{\alpha(\hat{a} + \hat{a}^\dagger)}{\sqrt{\sqrt{2}\lambda\alpha}}])^2 - \frac{2\lambda^2\alpha^2}{2}\frac{(\hat{a} + \hat{a}^\dagger)^2}{2\sqrt{2}\lambda\alpha} \tag{37}$$

and express the exponentials in a factorized normal form

$$\exp[\alpha(\hat{a} + \hat{a}^\dagger)] = e^{\alpha^2/2}\sum_{n=0}\sum_{k=0} \frac{\alpha^{n+k}\hat{a}^{\dagger n}\hat{a}^k}{n!k!}, \tag{38}$$

RWA on the above expression keeps only terms $n = k$, i.e. the double sum becomes a single sum, leading to Laguerre polynomials of order (operator) N. In this form we can recover equation (31) via RWA and using equation (37).

V. VALIDITY CHECK OF THE APPROXIMATION

In this section we numerically study the applicability of the above approximation as funtion of the system parameters.

A. Cosine potential

As pointed out, solutions of the Mathiue equation in closed analytical form do not exist. However, it is well known, from Floquet [30] and Bloch theory [31], that the spectrum of a periodic operator in 1-D is determined by a continouos quantum number k refered to as quasi momentum and a descrete number n called band index. The spectrum is most often represented within the first Brillouin zone [31] as allowed energy bands seperated by forbidden gaps. The characteristics of the spectrum are usually, in a phenomenological way, explained in two different ways; starting from a weak potential or a strong one. In the weak limit the particle is moving almost freely in a periodic background, which at the degenerate points split the degeneracy. In the oposite, strong potential limit, particles with energies smaller than the potential barriers will be quasi bound, and the tunneling rate determines the width of the bound energies, band width. As soon as a particle has an energy exceeding the barriers, it will move almost freely. Thus, we expect that the k-dependence is weak only for the lowest quasi bound energy bands when the amplitudes g_0 of the cosine potential is large. This is confirmed in fig. 1, which shows the lowest energy bands of the Mathiue equation for $q = 1$ and $g_0^2 = 10$.

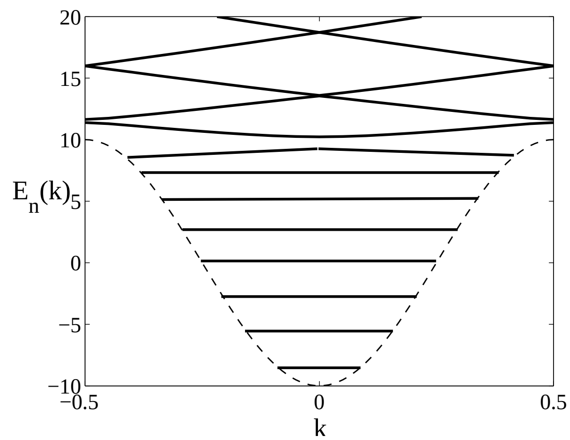

Figure 1: The spectrum $E_n(k)$, within the first Brillouin zone, of the Mathiue equation for a potential amplitude $g_0^2 = 10$ and wave number $q = 1$. The cosine function is plotted for clearity, showing that within the "wells" the particle is quasi bound.

The RWA is only supposed to work in the limit of $g_0 \gg q$, so it approximate only the lowest quasi bound energies. In fig. 2 we present the results of numerical calculations of the error estimete $\delta_E(n, g_0) = |E_n^{RWA} - E_n|$, where E_n^{RWA} is the approximate result for the energy from eq. (25),

$$E_n^{RWA} = g_0 q \left(n + \frac{1}{2}\right) - g_0^2 \left[\mathrm{e}^{-\frac{q}{4g_0}} L_n \left(\frac{q}{2g_0}\right) + \frac{q}{2g_0}\left(n + \frac{1}{2}\right) - 1\right] - g_0^2 \tag{39}$$

and E_n is the numerically calculated result of the energy by diagobnalization of the truncated Hamiltonian. Here the size of the Hamiltonian is 765×765 (well within the convergens limits for the eigenvalues). The reason why we show the absolute error, and not the relative one, is because for higher values of n, the energies become close to zero and the relative error fluctuates greatly in such cases. In the figure, the band index n runs between 0 and 5, hence showing the six lowest energies, and it is clear that the approximation breaks down for small couplings g_0 and high exitations n as expected.

B. Morse potential

As the Morse potential is analytically solvable, no numerical diagonalization of the Hamiltonian is needed. The bound energies for the Morse potential are [24, 25]

$$E_n = \sqrt{2}\lambda\alpha \left(n + \frac{1}{2}\right) - \frac{\alpha^2}{2}\left(n + \frac{1}{2}\right)^2. \tag{40}$$

Clearly, since $\lambda \gg \alpha$, the second anaharmonicity term becomes crucial only for larger excitations n. The anaharmonicity terms is purely negative resulting in that the highly excited bound states are more densly distributed. Interestingly,

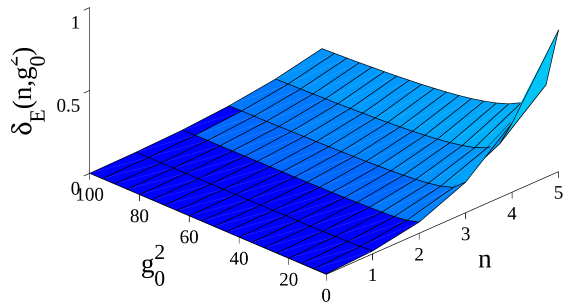

Figure 2: The absolute error $\delta_E(n, g_0^2) = |E_n^{RWA} - E_n|$, between the RWA result and the "exact" numerical result, as a funtion of the band index n and the amplitude g_0^2. The approximation is most valid for low excited bands n and strong couplings g_0. Again the wave number q is set to unity.

from the RWA result of eq. (36) we note that the second term is positive making the energies to be more sparse for high n's. However, this is partly compensated for by the coeffiecient 3/4 infront of the first harmonic part. It should be emphasized that only the even terms in the sums (32) are included since within the RWA odd terms vanishes. Thus, it is expected that the method may not be as efficient as for a situation with a purely even potential $V(x)$. It is more likely that the obtained eigenvalues approximate the ones for the Hamiltonian with a potential

$$\tilde{V}_{eff}(x) = \frac{V_{eff}(x)}{\lambda^2} = 1 + \sum_{k=0} \frac{(2\alpha x)^{2k}}{(2k)!} - 2\sum_{k=0} \frac{(\alpha x)^{2k}}{(2k)!}. \tag{41}$$

Using that $e^{x^2} = \sum_k \frac{x^{2k}}{k!}$, we expect that the potential (41) has some kind of "weak" exponential behaviour. In fig. 3 examples of the normalized effective potential $\tilde{V}_{eff}(x)/V_{eff}(1)$ are given for $\alpha = 0.1, 1$ and 10.

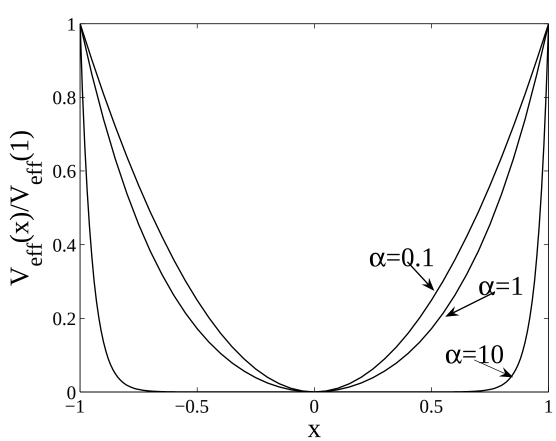

Figure 3: The normalized effective potential $\tilde{V}_{eff}(x)/V_{eff}(1)$ defined in eq. (41) for $\alpha = 0.1, 1$ and 10.

The relative error $\Delta_E(n, \lambda) = |E_n^{RWA} - E_n|/E_n$ between the expanded RWA result E_n^{RWA} (36) and the exact result E_n (40) is shown in fig. 4 for the first six eigenvalues and as a function of λ. In the plot $\alpha = 1$, but similar results are obtained for other widths α, however, with some increase of Δ_E for larger α.

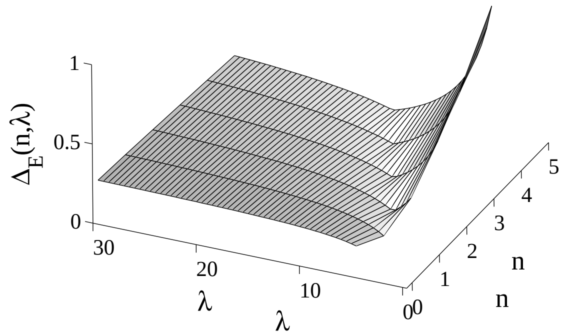

Figure 4: This plot displays the relative error $\Delta_E(n,\lambda) = |E_n^{RWA} - E_n|/E_n$ for $n = 0, 1, ..., 5$ and as a function of λ and here $\alpha = 1$.

VI. CONCLUSIONS

We have developed a method to approximate Hamiltonians using a kind of self-RWA. We have shown how some of the involved sums may be calculated using symmetrically ordered expressions for Fock-states expectation values of powers of the position operator.We have used these expressions to obtain approximations for Hamiltonians corresponding to the quantum rotor and the Morse potential. A discussion of the validity of the approximation was given and the relation with perturbation theory was explained. The direct link between first order perturbation theory and the RWA deepens the understanding of the two methods, and a consequent question would be if higher orders in the RWA scheeme could regain higher order perturbation theory. This seems possible, but has turned out to be more subtle than expected, mostly because of the non-commutability of the ladder operators.

Appendix A: CALCULATING SUMS VIA SYMMETRIC ORDER

In this appendix we use the results of the previous sections and show how one may use it to calculate various sums. Like in sectionII, no RWA is used and the results are exact.

We start with some function $f(x)$ which we can expand according to

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{2^{k/2} k!} \left(\hat{a}^\dagger + \hat{a}\right)^k . \tag{A1}$$

Here we have introduced the "symmetric" ladder operators $\hat{a}$ and $\hat{a}^\dagger$ obeying the regular boson commutator algebra $[\hat{a}, \hat{a}^\dagger] = 1$ and which are related to $\hat{x}$ and $\hat{p} = -i\frac{\partial}{\partial x}$ as

$$\begin{aligned} \hat{x} &= \tfrac{1}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right) \\ \hat{p} &= \tfrac{i}{\sqrt{2}}\left(\hat{a}^\dagger - \hat{a}\right). \end{aligned} \tag{A2}$$

Further we have the normalized eigenstates and eigenvalues of the number operator $\hat{N} = \hat{a}^\dagger \hat{a}$; $\hat{N}|n\rangle = n|n\rangle$, where $n = 0, 1, 2, ...$, and which in x-basis are

$$\Psi_n(x) = \langle x|n\rangle = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} \mathrm{e}^{-x^2/2} H_n(x). \tag{A3}$$

As argued in section II, the diagonal elements, in the Fock basis, of the function $f(x)$ is identical to the diagonal elements of the function $\tilde{f}(\hat{x}, \hat{p})$ where only terms containing an equal number of creation and annihilation operators are included. We thus have

$$\langle n|\tilde{f}|n\rangle = \langle n|f|n\rangle. \tag{A4}$$

The L.H.S. can be written, using equation (10), as

$$\tilde{f} = \sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{f^{(2j+2l)}(0)}{2^j (2!)^2} \frac{N!}{(N-j)!} \tag{A5}$$

and if we express the R.H.S. in the x-basis we obtain

$$\sum_{l=0}^{\infty} \frac{1}{2^{2l} l!} \sum_{j=0}^{\infty} \frac{V^{(2j+2l)}(0)}{2^j (j)!^2} \frac{n!}{(n-j)!} = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{+\infty} V(x) \mathrm{e}^{-x^2} H_n^2(x) dx, \tag{A6}$$

Below we give some analytically solvable examples. Approximate results is in principle easily achievable, but is left out in this paper.

1. Cosine function

For a cosine function $V(x) = \cos(qx)$ we have $V^{(2k)}(0) = (-1)^k q^{2k}$ and we find [32] in (A6)

$$\begin{aligned} \text{L.H.S.} &= \sum_{l=0}^{\infty} \frac{(-1)^l q^{2l}}{4^l l!} \sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!} = \mathrm{e}^{-\frac{q^2}{4}} \sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!} \\ \text{R.H.S.} &= \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{+\infty} \cos(qx) \mathrm{e}^{-x^2} H_n^2(x) dx = \mathrm{e}^{-\frac{q^2}{4}} L_n(q^2/2). \end{aligned} \tag{A7}$$

So that

$$\sum_{k=0}^{\infty} \frac{(-1)^k q^{2k}}{2^k (k!)^2} \frac{n!}{(n-k)!} = L_n(q^2/2). \tag{A8}$$

Note that closed forms of $V(x) = \exp(\pm iqx)$, $V(x) = \cosh(qx)$, $V(x) = \cosh^m(qx)$ or $V(x) = \cos^m(qx)$, $m = 0, 1, 2, ...$ can also be obtained.

2. Gaussian function

In the case of $V(x) = \exp\left(-\alpha^2 x^2\right)$, $\alpha^2 > 0$, the integral in the R.H.S. of eq (A6) is analytically solvable [32]

$$\frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\alpha^2 x^2} \mathrm{e}^{-x^2} H_n^2(x) dx = 2^{n+1} \left(\frac{2\alpha^2}{\alpha^2 + 2} \right)^{n+1/2} \frac{\alpha^{-1}}{n} F\left(-n, n; -\frac{2n-1}{2}; \frac{\alpha^2 + 2}{2\alpha^2} \right), \tag{A9}$$

where $F(..., ...; ...; ...)$ is the Gauss hypergeometric function. The derivatives are simply $V^{(2k)}(0) = (-1)^k \alpha^{2k} \frac{k!}{(2k)!}$ resulting in the L.H.S.

$$\text{L.H.S.} = \sum_{l=0}^{\infty} \frac{(-1)^l \alpha^{2l}}{4^l l!} \sum_{j=0}^{\infty} \frac{(j+l)!}{(2j+2l)!} \frac{(-1)^j \alpha^{2j}}{2^j (j)!^2} \frac{n!}{(n-j)!}. \tag{A10}$$

The above holds also for exponential functions such that $0 > \alpha^2 > -1$, which, when applied to Hamiltonian systems, is of interst as they possess an infinite set of bound states.

3. Hermite polynomials

When $V_m(x) = H_{2m}(x)$, where $m = 0, 1, 2, ...$ we find [32]

$$\text{R.H.S.} = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{+\infty} H_{2m}(x) \mathrm{e}^{-x^2} H_n^2(x) dx = \frac{2^{m/2} m! n!}{\left(\frac{m}{2}!\right)^2 \left(n - \frac{m}{2}\right)!}, \tag{A11}$$

while its derivatives are $V_m^{(2k)}(0) = \frac{2^{2k}(2m)!}{(2k)!} H_{2m-2k}(0)$.

ACKNOWLEDGMENTS

J. L. acknowledges Prof. M. Lewenstein, EU-IP Programme SCALA (Contract No. 015714) and the Swedish Goverment/Vetenskapsrådet for financial support. H. M.-C. acknowledges E. Kajari for useful discussions and the Alexander von Humboldt for support.

[1] I. I. Rabi, Phys. Rev. **49**, 324 (1926); **51**, 652 (1937).

[2] L. Allen and J. H. Eberly, *Optical Resonance and Two-level Atoms* (Dover Publications, 1087)

[3] L. Mandel, and E. Wolf, *Optical Coherence and Quantum Optics*, (Cambridge University Press, 1995).

[4] E.T. Jaynes and F.W. Cummings, Proc. IEEE **51** 81 (1963).

[5] B. W. Shore, and P. L. Kn ight, J. Mod. Opt. **40**, 1195 (1993).

[6] A. Messina, S. Maniscalo, and A. Napoli, J. Mod. Opt. **50**, 1 (2003).

[7] D.J. Wineland, C. Monroe, D.M. Meekhof, B.E. King, D. Leibfried, W.M. Itano, J.C. Bergquist, D. Berkeland, J.J. Bollinger and J. Miller, Proc. of the Royal Soc. of London Series A 454, 411 (1998); F. Schmidt-Kaler, H. Haffner, M. Riebe, S. Gulde, G. P. T- Lancaster, T. Deuschle, C. Becher, C. F. Roos, J. Eschner, and R. Blatt, Nature **422**, 408 (2003).

[8] H. Walther, B. T. H. Varcoe, B. G. Englert, and T. M. Becker, Rep. Prog. Phys. **69**, 1325 (2006); Brune,S. Haroche,J. M. Raimond,L. Davidovich, and N. Zugary, Phys. Rev A bf 45, 5193 (1992); C. J. Hood, T. W. Lynn, A. C. Doherty, A. S. Parkins, and H. J. Kimble, Science **287**, 1447 (2000);

[9] K. Bergmann, H. Theuer, and B. W. Shore, re. Mod. Phys. **70**, 1003 (1998).

[10] K. Zaheer, and M. S. Zubairy, Phys. Rev. A **37**, 1628 (1988); K. Zaheer, and M. S. Zubairy, Opt. Commun. **73**, 325 (1989); M. D. Crisp, Phys. Rev. A **43**, 2430 (1991); J. S. Peng, and G. X. Li, Phys. Rev. A **45**, 3289 (1992); R. F. Bishop, N. J. Davidson, R. M. Quick, and D. M. van der Walt, Phys. Rev. A **54**, R4657 (1996); M. F. Fang, and P. Zhou, Physica A **324**, 571 81996).

[11] F. Bloch, and A. Siegert, Phys. Rev. **57**, 522 (1940).

[12] G.B. Arfken and H.J. Weber,*Mathematical Methods for Physicists* (Academic Press, 2001).

[13] K. Fujii and T. Suzuki, Mod. Phys. Lett. A **19**, 827 (2004).

[14] J. C. Guiterrez-Vega, *Theory and numerical analysis of the Mathieu functions*, http://homepages.mty.itesm.mx/jgutierr/Mathieu/Mathieu.pdf

[15] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[16] J. C. Guiterrez-Vega, R. M. Rodriguez-Dagnino, M. A. Meneses-Nava, S. Chavez-Cerda (2003), Mathieu functions, a visual approach, Am. J. Phys. **71**, 3.

[17] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. rev. Lett. **81**, 3108 (1998); D. jaksch, and P. Zoller, Ann. Phys. **315**, 52 (2005); M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen De, and U. Sen, arXiv: quant-ph/0606771.

[18] D. Frenkel and R. Portugal, J. of Phys. A **34**, 3541 (2001).

[19] D. J. J. O'Dell, *Dynamical diffraction in sinusodial potentials: uniform approximations for Mathieu functions*, J. Phys. A: Math. Gen. **34**, 3897 (2001).

[20] C. A. Dartora, K. Z. Nobrega and H. E. Hernandez-Figueroa (2005), New analytical approximations for the Mathieu functions, Appl. Math. Comp. **165**, 447.

[21] L. Esaki, and L. L. Chang, Phys. Rev. Lett. **33**, 495 (1974); D. L. Smith, and C. Mailhiot, Rev. Mod. Phys. **62**, 173 (1990).

[22] L. Guidoni, and P. Verkerk, Phys. Rev. A **57**, R1501 (1998); S. Peil, J. V. Porto, B. L. Tolra, J. M. Obrecht, B. E. King, M. Subbotin, S. L. Rolston, and W. D. Phillips, Phys. Rev. A **67**, 051603 (2003).

[23] J. J. Sakurai, *Modern Quantum Mechanics*, (Addison Wesley, 1994).

[24] P. M. Morse, Phys. Rev. (1929), **34** 57.

[25] L. D. Landau and E. M. Lifshitz 1977, Quantum Mechanics (Nonrelativistic Theory) (Oxford: Pergamon)

[26] P. Atkins and R. Friedman, Molecular Quantum Mechanics, (Oxford University Press, 2005)

[27] I. A. Ivanov (1997) WKB quantization of the Morse Hamiltonian and periodic meromorphic functions. J. Phys. A: Math. Gen. **30**, 3977.

[28] V. G. Romanovski and M. Robnik (2000), Exact WKB expansion for some potentials, J. Phys. A: Math. Gen. **33**, 8549.

[29] I. L. Cooper, J. Phys. A: Math. Gen. **26**, 1601 (1993); M. G. Benedict, and B. Molinr, Phys. Rev. A **60**, R1737 (1999);

[30] G. Floquet, *Sur les équations différentielles linéaires à coefficients périodiques*, Ann. École Norm. Sup. **12**, 47-88 (1883); J. E. Bayfield, *Quantum Evolution*, (John Wiley & Sons, 1999).

[31] F. Bloch, *Über die Quantenmechanik der Elektronen in Kristallgittern*, Z. Physik **52**, 555-600 (1928); C. Kittel, *Quantum Theory of Solids*, (John Wiley & Sons, 1987).

[32] I. S. Gradshteyn and I. M. Ryzhik 2000, Table of integrals, series and products, (Academic Press).